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Electron-electron interaction in a two-dimensional electron gas: Bound states at low densities

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If the bare interaction between two electrons is dressed in the two-dimensional electron gas by the response of the many-body environment, pairing may occur. Here, we study numerically the existence and character of bound states in the case where the dressing in the pair-interaction energy is described by the Overhauser geminal model [A. W. Overhauser, Can. J. Phys. **75**, 683 (1995)]. The starting point of the model is the exchange correlation hole around a single electron. We constrain the hole by arguments based on the results for the exchange-correlation energy and the contact density of the pair-correlation function. We find a bound state with the energy minimized at a certain electron gas density. On the basis of the behavior of the binding energy we discuss recent experimental findings for the electron density dependence of the critical temperature in cuprate, Chevrel-phase, and Li-intercalated Li_xZrNCl superconductors.

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I. INTRODUCTION

Strongly correlated two-dimensional (2D) electron systems offer a rich phenomenology raising theoretical interest in the role of reduced dimensionality with Coulomb forces between fermions and a practical interest in possible technological applications. Maybe the most important phenomenon is the competition between electrostatic and kinetic energies in the quantum range. Within the idealized model of a 2D homogeneous electron gas and charge-compensating rigid background the competition leads to different phases, such as unpolarized and polarized liquids,[1–3] possible intermediate states,[4–6] and the Wigner crystal.[7–10]

In this work we are interested in a possible Cooper channel with effective electron-electron attraction in 2D. This pairing has been discussed explicitly by Randeria *et al.*[11] using a qualitative model for pair interaction and by Ghazali and Gold[12] applying a dielectric screening to model an effective potential. A Cooper channel other than the conventional phonon-mediated attractive interaction between electrons seems necessary in order to understand the measured trends in the critical temperature of cuprate, Chevrel-phase, and Li_xZrNCl superconductors.[13,14] Moreover, this kind of channel could explain the recent finding of a bosonic contribution to the thermal conductivity of underdoped $YBa_2Cu_3O_x$.[15] Recent success using the geminal representation for a correlated-*pair* state and different effective pair potentials[16–20] to calculate associated pair-correlation functions has motivated a further study on the possibility of pairing in 2D. As the onset of superconductivity is related to some form of increased order in the motion of the electrons, it is necessary, therefore, to take into account *ways* in which electrons interact with each other.[21]

Briefly, the motivating attempts[16–20] are based on properly weighted positive-energy scattering states (below the Fermi energy) needed to construct pair correlation functions. The success achieved suggests a similar attempt in the negative-energy, bound-state region of the pair interaction. The physical picture behind the pair-correlation function governs a path on which a consistent pair-potential construction can be based. We apply, from these attempts, the screened-electron-screened-electron model[20] to construct a pair potential $V_{ee}(R)$ which describes the relative movement of two electrons in their host system. In the present work we constrain our model by pair-correlation and energetic arguments. By a numerical solution of the ensuing effective one-particle Schrödinger equation we find a bound state, the energy eigenvalue of which is minimized at a certain low electron density.

Of course, showing the possibility of bound pair states in an effective two-body potential is only a first step. Other arguments[11] and further many-body efforts are needed to achieve a definite statement on the physical reality of superconductivity in 2D.

II. MODEL AND RESULTS

In the geminal representation we consider a pair of electrons with antiparallel spins and model the screening density, superimposing[20] normalized Gaussian charges

$$\Delta n(r) = (\beta^2/\pi)\exp(-\beta^2 r^2), \tag{1}$$

centered around *both* electrons. The statistical and dynamical correlations are encoded in a normalized hole.[21] The value of β will depend on the 2D electron density $n_0 = 1/(\pi r_s^2)$, and it will be constrained below. The screened-electron-screened-electron electrostatic interaction energy for the interelectron distance of R can be obtained in our symmetric model most easily as a convolution of quantities in the wave-vector (q) space:

$$V_{ee}(R) = \frac{1}{2\pi}\int_0^\infty dqqJ_0(qR)V_{ee}(q)$$

$$= \frac{1}{2\pi}\int_0^\infty dqqJ_0(qR)[1-\Delta n(q)]\frac{2\pi}{q}[1-\Delta n(q)]. \tag{2}$$

Here $J_0(x)$ is the zeroth-order Bessel function and $\Delta n(q) = \exp[-q^2/(2\beta)^2]$ is the Fourier-Hankel transform of the Gaussian screening density of Eq. (1).

The above informative representation for $V_{ee}(q)$ shows that $V_{ee}(q \to 0) \sim q^3$. Thus, $V_{ee}(R)$ belongs to the class of circularly symmetric potentials obeying

$$\int_0^\infty 2\pi r dr V(r) = 0. \tag{3}$$

This class of potentials was investigated by Simon[22] who proved the theorem that a not-everywhere non-negative effective potential $\Lambda V(r)$ has a bound state for *all* $\Lambda \neq 0$. The existence of the bound state is the mathematical basis of our present study.

At this point we notice an important fact, which is related to the physical reality of the present potential construction. In 2D, one defines a Friedel-like sum[23]

$$S(2\mathrm{D}, k_r) = \frac{2}{\pi} \sum_{m=-\infty}^{\infty} \eta_m(k_r) \tag{4}$$

of scattering phase shifts $\eta_m(k_r)$. In the present case k_r is the relative momentum in the center-of-mass system of two distinguishable particles. In our model, the first-order Born approximation gives $S(2\mathrm{D}, k_r) = 0$ because $S(2\mathrm{D}, k_r) \sim V_{ee}(q=0)$, perturbatively.[24] Consequently, no new excess charge or change in the associated spectral density[25] is generated; we have only distortion[26] in the density profile due to interactions. Due to this fact, the competing kinetic energy-density *change*, which is mediated by pair interactions (collisions),[27,28] also vanishes, since it is proportional to the product of the density n_0 of the uniform 2D electron gas and $V_{ee}(q=0)$.

By performing the integration in the above Equation (2), we obtain

$$V_{ee}(R) = \frac{1}{R} - 2\frac{1}{R}\sqrt{2\pi z} I_0(z) e^{-z} + \frac{1}{R}\sqrt{\pi z} I_0(z/2) e^{-z/2}, \tag{5}$$

where the shorthand $z = \beta^2 R^2/2$ is introduced and I_0 is the modified Bessel function. The effective potential is repulsive at short distances and diminishes as $+[9/(16\beta^4 R^5)]$ for $R \to \infty$. The shielding function $F(z) \equiv R V_{ee}(R)$ is shown in Fig. 1 for the range $z \in [0, 10]$. A negative minimum appears at about $z = 0.5$, heralding the optimal value $\beta R \approx 1$. We note that a quite similar *shape* for the 2D effective interaction was obtained by Khalil *et al.*[29] by using a many-body method based on polarization and fluctuational diagrams. Remarkably, they also suggested that this kind of effective potential may have a possible role in superconductivity.

In our model we have to constrain the parameter $\beta(r_s)$. We outline two options in order to motivate our final simple choice $\beta(r_s) = 1/r_s$ for the low densities of the 2D electron gas at which the binding of the two electrons is optimal. In the first option we consider the interaction energy $\varepsilon_{int}(r_s)$ (Ref. 30) of an electron with its screening hole—i.e.,

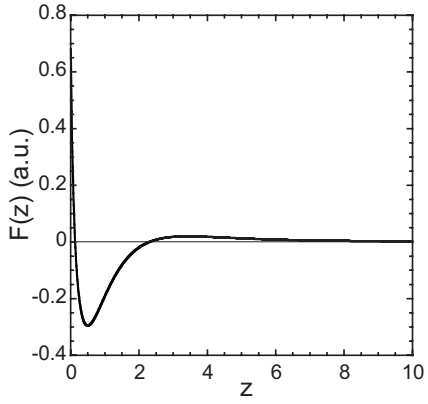

FIG. 1. The shielding function $F(z)$ defined in the text, as a function of $z = \beta^2 R^2/2$.

$$\varepsilon_{int}(r_s) = -\frac{1}{2} 2\pi \int_0^\infty dr r \frac{1}{r} \Delta n(r, \beta) = -\frac{\beta\sqrt{\pi}}{2}. \tag{6}$$

This can be related to the exchange-correlation energy $\varepsilon_{xc}(r_s)$ of the 2D electron gas. By using for $\varepsilon_{xc}(r_s)$ the Padé interpolation form[1] based on the data (for $r_s \in [1, 20]$) of Monte Carlo calculations results in $r_s \beta(r_s) > 1$ for $r_s > 8$; for example, at $r_s = 20$ one has $r_s \beta(r_s) \approx 1.07$. This means that the change in the contact electron density due to the exchange-correlation hole, in our model $\Delta n(r=0) = (\beta^2/\pi)$, would be slightly larger than the uniform density $n_0 = 1/(\pi r_s^2)$, which is unphysical in principle.

The second option, which is also tied to two-body physics, could rest on recent results[31] for the on-top values $g(r=0, r_s)$ of the average pair-correlation function. They should equal the values of our screening hole at the origin—i.e., $g(0, r_s) = 1 - |\Delta n[r=0, \beta(r_s)]|/n_0$. At low densities this constraint for $\beta(r_s)$ would lead to the approach of the total charge depletion limit $\beta(r_s) \to 1/r_s$ from below, because of the small finite $g(0, r_s)$ values. Figure 2 of Ref. 31 shows that $g(0, r_s)$ is very close to zero already at $r_s = 5$ [$g(0, r_s = 5) < 0.02$].

The two above options bracket at low electron densities the total charge depletion case $\beta(r_s) = 1/r_s$, which shall therefore be our practical choice. This choice results only in a weak violation of the equality $\varepsilon_{int}(r_s) = \varepsilon_{xc}(r_s)$. At $r_s = 5$ one gets $\varepsilon_{int}(r_s) \approx -0.17$ hartree while $\varepsilon_{xc}(r_s) \approx -0.15$ hartree. At $r_s = 20$ we have $\varepsilon_{int}(r_s) \approx -0.044$ hartree while $\varepsilon_{xc}(r_s) \approx -0.047$ hartree. The deviations are small which, together with the above analysis on distortion and a negligible kinetic-energy change, suggest that our one-parameter model is physically well optimized already from about $r_s \approx 5$. With our choice for $\beta(r_s)$ the important minimum in the residual interaction appears at $R \approx r_s$. We have thus, via the residual form, a picture of the combined effects[32] of averaging, screening, and correlating which affect the net interaction, similarly as in Landau's theory for quasiparticle-quasiparticle interactions.

Now when we have fixed the interaction potential $V_{ee}(R)$ for different r_s values we turn our attention to the determination of the bound-state energy E_b and corresponding wave

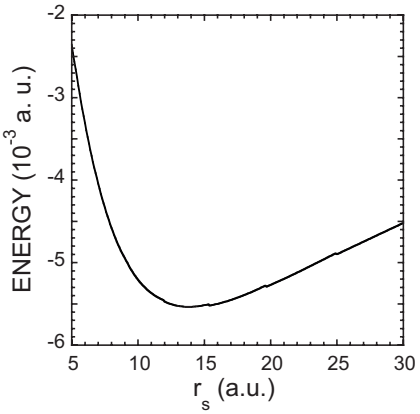

FIG. 2. Binding energies $E_b(r_s)$ in the screened electron-electron potential of Eq. (5). The energies are solutions to Eq. (9) with the effective mass $\mu=0.5$.

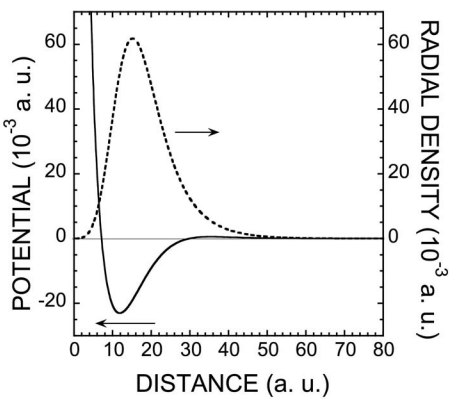

FIG. 3. The radial density $2\pi R|\Psi(R)|^2$ and the electron-electron screened potential for the optimal value of $r_s=13.9$.

function $\psi(R)$ of the two-electron system. We solve numerically[30] the 2D Schrödinger equation

$$\left[-\frac{1}{2\mu}\nabla^2 + V_{ee}(R) - E_b\right]\psi(R) = 0, \tag{7}$$

where $\mu=1/2$ is the reduced mass. In circular symmetry the wave function separates in the standard manner as

$$\psi(R) = \frac{e^{im\phi}}{\sqrt{2\pi}}U_{mn}(R), \tag{8}$$

in which $m=0,\pm1,\pm2,\ldots$ is the azimuthal quantum number and $n=1,2,3,\ldots$ is the radial quantum number related to the number of radial nodes $(n-1)$ of the radial wave function $U_{mn}(R)$. In this work we are interested in the ground state $n=1$ and $m=0$. By making the substitution $u_{mn}(R)=R^{1/2}U_{mn}(r)$ we obtain the differential equation

$$\frac{d^2u_{mn}(R)}{dR^2} + \left(2\mu[E_b - V_{ee}(R)] - \frac{(m^2-1/4)}{R^2}\right)u_{mn}(R) = 0. \tag{9}$$

This is the same form as the radial equation studied in spherically symmetric problems. We solve the equation on an exponentially expanding radial mesh, $R(j)=r_{min}\exp[(j-1)\Delta x]$, with $j=1,\ldots,N$. With a given guess for the eigenenergy E_b the function $u_{mn}(R)$ is integrated outwards from the origin and inwards from a large radius by starting with its asymptotic expansion. At a matching point close to the classical turning point the logarithmic derivatives of the outward and inward integrated solutions are required to coincide by adjusting the eigenvalue E_b. The parameters of the radial mesh, R_{min}, Δx, and N, are varied until numerical convergence of the eigenvalue is obtained.

By using $\beta(r_s)=1/r_s$ we calculate the binding energies E_b from Eq. (9) with the potential of Eq. (5). The results are shown in Fig. 2 as a function of the density parameter r_s. The binding energy increases rapidly with increasing r_s, attains a minimum around $r_s\approx13.9$, and decreases thereafter slowly towards lower electron densities. The radial density $2\pi R|\psi(R)|^2$ corresponding to the energy minimum is exhibited in Fig. 3. The density is fairly localized, due to the well-like nature of the circular $V_{ee}(R)$.

Finally, in the light of the binding energy versus the r_s-parameter curve in Fig. 2 we discuss the behavior of the critical temperature (T_c) measured for cuprate and Chevrel-phase superconductors[13] as well as for the Li-intercalated (Li-doped) Li_xZrNCl superconductor.[14] In these materials the conduction electrons can be thought to form a 2D electron gas. According to Uemura *et al.*,[13] T_C increases in the cuprate and Chevrel-phase superconductors as a function of the increasing charge carrier density until it saturates and is eventually suppressed. From a similar parabolic dependence (Uemura plot) of the transition temperature on condensate density *universal* trends, based on experimental results, has been concluded and the crucial constraining role of these trends on the microscopic theory has been pointed out.[33] This behavior can be understood if we assume, as a first approximation,[34] that T_C is proportional to the binding energy E_b of the electron pair. Then the increase of T_C means the approach of the energy minimum from the side of the high-r_s values and the saturation and suppression would signal the passing of the energy minimum. The 2D charge-carrier densities giving the maximum T_C values in Fig. 3 of Ref. 13 are around $0.66n_0(m_e/m^*)\approx5\times10^{13}$ cm^{-2}. From this and based on the assumption $m^*=m_e$, one gets $r_s\approx12$ a.u. $[n_0=1/(\pi r_s^2)]$, which is indeed in the optimal range in our Fig. 2.

Taguchi *et al.*[14] measured T_C for the Li_xZrNCl superconductor as a function of the Li doping x. They were able to reduce x down to the occurrence of the insulator phase at $x=0.05$ and keeping the Li intercalation uniform without phase separation. T_C showed a strong increase when x decreased from 0.12 to 0.06, corresponding to the increase of the 2D r_s parameter from 7.3 to 10.3. Again, assuming that T_C is proportional to E_b the increase in T_C is in agreement with the strong increase in the binding energy from the low-r_s values toward the minimum energy at around $r_s\approx13.9$. At higher Li concentrations $0.12<x<0.31$, T_C increases moderately with decreasing x. The switching to this behavior may signal the gradual domination of the electron-phonon interaction in the electron pairing with increasing electron density. We notice that in a special two-band model of me-

tallic (three-dimensional) hydrogen[35] the density dependence of T_c, without phonons, resembles our findings above; the dependence heralds increasing T_c with decreasing electron gas density.

III. SUMMARY AND COMMENTS

We have pointed out the possibility of pairing of two electrons in the 2D fermionic environment by using an effective pair interaction to their relative motion. The study performed complements earlier[11,12] and more recent[30] attempts in this field and provides a reasonable physical picture to the rich phenomenology of strong correlation effects. The basis of our model is the charge depletion around an electron. We estimate it in a physically reasonable way which is valid also within the important low-density range. However, the most important ingredient to the existence of the bound state for the two electrons is the oscillating nature of the effective interelectron potential. This oscillation is behind the minimum nature of the kinetic energy change, also.

The problem of how our results can appear at the total wave-function level needs further attempts. The question of necessary *and* sufficient conditions was already investigated by stating[11] that the many-body ground state is unstable to pairing if and only if a two-body bound state exists. Thus the possible existence of a bound state in a consistently constrained effective interaction implies the nontrivial problem related to a *self*-consistent construction of the pair-correlation function in a geminal model; such a construction also needs future considerations.

In order to demonstrate the importance of our results in a physical case we discussed the behavior of the critical temperature in superconductors where the charge carriers can be thought to form a 2D electron gas. The attractive electron-electron interaction with the energy minimun at $r_s \approx 13.9$ can account for the experimental findings in contrast to the conventional phonon-mediated interaction.

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